

Pair Wave Functions in a Bose Liquid

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Pair wave functions (PWF) which are eigenfunctions of the reduced density 2-matrix are considered for a homogeneous Bose liquid. With the Bogoliubov principle of the correlation weakening it is proved that the distribution of the “dissociated” pair states over momenta is exactly the product of the single-particle distribution functions. Thus, the “dissociated” pair states are naturally classified as condensate-condensate, condensate-supracondensate and supracondensate-supracondensate ones provided the Bose-Einstein condensate exists. The condensate-condensate as well as condensate-supracondensate PWF are expressed in terms of the averages of products of the creation and destruction Bose operators. This leads to the simple interpretation of the anomalous averages as the “scattering parts” of the condensate-condensate and condensate-supracondensate PWF. It is shown that in contrast to the Fermi liquid, the appearance of the anomalous averages for the Bose liquid does not necessarily mean that there exist bound states of pairs of particles. The PWF in the Hartree-Fock-Bogoliubov (HFB) approach are found. Given the density of the condensate is not zero, there are no bound pair states in the HFB scheme. The expansion of the pair correlation function in the set of PWF is very useful in order to take into account both short-range and long-range spatial correlations. Applications (possible and already realized) of the formalism developed are discussed.

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I. INTRODUCTION

It is well-known that for the homogeneous Fermi liquid the appearance of anomalous averages $\langle \hat{\psi}^\dagger(x_1)\hat{\psi}^\dagger(x_2) \rangle$ implies that there exists a macroscopic number of bound pairs of particles with zero momentum (here $\hat{\psi}^\dagger(x)$ and $\hat{\psi}(x)$ are the field operators). In the case of the pair condensate like this, the properties of the system change radically. In particular, this leads to the superfluidity of the Fermi liquid (superconductivity in an electron system, superfluidity in ^3He).

For a homogeneous Bose liquid, the superfluidity is usually associated with the macroscopic number of particles themselves in the zero-momentum state (the Bose-Einstein condensate). In the Bogoliubov theory for a weakly imperfect Bose gas, repulsive interaction between particles depletes the condensate, while makes it thermodynamically stable. In this case the anomalous averages $\langle \hat{\vartheta}^\dagger(\mathbf{r}_1)\hat{\vartheta}^\dagger(\mathbf{r}_2) \rangle$ play a crucial role also, where $\hat{\vartheta}^\dagger(\mathbf{r})$ is the field operator creating a supracondensate particle at a point \mathbf{r} , see Eq. (34).

Parallels between the Bogoliubov transformations for boson [1] and fermion [2] systems gave birth to pair theories being special cases of the HFB theory (see, e.g. Ref. [3] and references therein). In the framework of the HFB approach, the gap in the single-particle excitation energy appears [4] that may be interpreted, by analogy with the theory of superconductivity, as an evidence for the bound states of pairs of particles. Below we show that in the presence of a single-particle condensate, there are no bound pair states of bosons in the HFB theory. Thus, it has been verified in terms of PWF that the gap is unphysical, which has been stressed in many papers [4,5].

The concept of wave functions for a group of m particles in medium can be rigorously introduced with eigenfunctions of the m -th-order reduced density matrix, or the m -matrix. Indeed, the system of m particles is a subsystem of that of N particles. So, its state is not pure even in the situation when the system as a whole has a wave function. In general a subsystem is specified by the density matrix (see, e.g. Ref. [6]). The m -matrix is of use when we have a noncoherent superposition of the m -particle wave functions. Löwdin and Shull used wave functions like these for one and two particles to describe electron states in atoms, and called them the “natural orbitals” and “natural geminals”, respectively (see Ref. [7]). The concept of PWF for fermions has been used by Shafroth and his coworkers in papers on the theory of superconductivity (for a review, see Ref. [8]). In what follows, we shall use the term PWF for the wave functions of particle pairs, using the notation of Bogoliubov who made the most clear presentation of the concept of PWF for fermions [9].

This paper concerns PWF for the Bose liquid below the temperature of the condensation, T_c . Analysis is carried out in general form as far as it is possible, with a special emphasis on the bound pair states and that part of PWF which is responsible for the correlations of particles at short distances. Consideration of these correlations is of special interest when investigating concrete boson systems for which the potential of two-particle interaction $\Phi(r)$ is, as a rule, strongly singular, or, in other words, of the hard-core type (i.e. potential goes to infinity like $1/r^m$ ($m > 3$) as $r \rightarrow 0$, and, consequently, there is no Fourier transform of it). For example, the well-known Lennard-Jones potential is of this form. In

this case standard approximations based on the weak-coupling perturbation theory lead to divergencies. For example, the statistical average of the interaction energy per particle

$$\varepsilon_{int} = \frac{1}{N} \left\langle \frac{1}{2} \sum_{i \neq j} \Phi(|\mathbf{r}_i - \mathbf{r}_j|) \right\rangle = \frac{n}{2} \int d^3r \Phi(r) g(r) \quad (1)$$

(here $g(r)$ is the pair distribution function, n is the density of the particles) is infinite in the simplest Hartree approximation corresponding to $g(r) = 1$. A reason for the divergency is obvious as the short-range spatial correlations of two particles are not properly taken into consideration. In order to escape the mentioned trouble a real potential is usually replaced by various effective potentials for which the Fourier transforms exist (for the Bose case see the t -matrix approach [10], the pseudopotential with positive scattering length, or the hard-sphere model, [11] and the method by Beliaev [12]). This replacement implies that the effective potential contains all “information” on the short-range correlations of particles. A range of validity of this replacement for the many-boson systems is discussed in the textbook [13] and, for an inhomogeneous gas, in the recent paper [14] (see the discussion at the end of Sec. IV). In the lowest order in density n of the Bose gas such effective-interaction procedures are reduced to the Bogoliubov model with the effective potential [for example, in the pseudopotential method the Fourier transform of the “bare” potential is replaced by $\Phi(k) = 4\pi a/m$, where a is the scattering length obtained from the two-body Schrödinger equation]. However, this approach is found to be thermodynamically inconsistent [15], which can manifest itself in various unphysical results. For example, one can obtain no depletion of the Bose condensate within the pseudopotential approach, if one tries to apply a self-consistent treatment [16]. Besides, we are not able to obtain the correct value of the interaction energy (1) by direct calculations using $g(r)$ [17]. Thus, it looks interesting and promising to realize an alternative variational scheme that is self-consistent from the very beginning, as the short-range correlations are properly taken into account for all the terms in the expansion of $g(r)$ (31) in the set of PWF. Thus, PWF are “regular channels” which can be used to cancel the divergencies in a self-consistent manner (see discussion in Secs. IV and V). The first results derived in Refs. [15,18,19] demonstrate that the formalism of the PWF can actually be employed as a basis for the self-consistent variational treatment for a Bose gas with the strongly singular interaction potential.

General properties of the eigenfunctions and eigenvalues of the correlation function (5) (differing from the 2-matrix only by a norm) are interesting in itself when an eigenvalue becomes a macroscopic quantity (off-diagonal long-range order [20]). With the Bogoliubov principle of correlation weakening we shall show that eigenvalues of the correlation function (5) which belong to continuous spectrum (“dissociated” pair states) are expressed as the

product of the single-particle momentum distributions. Thus, the “dissociated” pair states are naturally classified as condensate-condensate, condensate-supracondensate and supracondensate-supracondensate ones provided the Bose-Einstein condensate exists. The condensate-condensate as well as condensate-supracondensate PWF are expressed in terms of the averages of products of the creation and destruction Bose operators. This leads to the simple interpretation of the anomalous averages as the “scattering parts” of the condensate-condensate and condensate-supracondensate PWF (see Sec. III).

In the next section, the PWF are introduced for boson systems by analogy with Bogoliubov’s paper [9], and the continuous spectrum of the correlation function (5) is calculated. In Sec. III we consider the general structure of the 2-matrix below T_c , the PWF in an explicit form and their physical interpretation. In Sec. IV the PWF are evaluated in HFB approach as well as in the Bogoliubov model, and some applications of the developed formalism are considered. Main results are summarized in Sec. V.

II. THE CONCEPT OF PARTICLE PAIR STATES FOR BOSONS

Let us consider a homogeneous system of N bosons, and, for simplicity, let the spin of the particles be equal to zero. The Hamiltonian is assumed to be invariant with respect to translations and the transformation of particle momentum $\mathbf{p}_i \rightarrow -\mathbf{p}_i$. The latter implies that the Hamiltonian does not change when the canonical transformation $\hat{a}_{\mathbf{k}} \rightarrow \hat{a}_{-\mathbf{k}}$, $\hat{a}_{\mathbf{k}}^\dagger \rightarrow \hat{a}_{-\mathbf{k}}^\dagger$ is performed. In particular, this condition is satisfied for pairwise interactions with a potential $\Phi(\mathbf{r}) = \Phi(r)$. A state of the system is determined by a density matrix

$$\rho(\mathbf{r}'_1, \dots, \mathbf{r}'_N; \mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_n w_n \Psi_n^*(\mathbf{r}_1, \dots, \mathbf{r}_N) \times \Psi_n(\mathbf{r}'_1, \dots, \mathbf{r}'_N), \quad (2)$$

where $\sum_n w_n = 1$, $w_n \geq 0$, and Ψ_n are orthonormal system of functions being symmetric with respect to any permutations of particles.

The 2-matrix is defined as

$$\rho_2(\mathbf{r}'_1, \mathbf{r}'_2; \mathbf{r}_1, \mathbf{r}_2) = \int_V d^3r_3 \dots d^3r_N \times \rho(\mathbf{r}'_1, \mathbf{r}'_2, \mathbf{r}_3, \dots, \mathbf{r}_N; \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N), \quad (3)$$

and can be expressed in terms of the field operators $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$ (see, e.g. Ref. [21])

$$\rho_2(\mathbf{r}'_1, \mathbf{r}'_2; \mathbf{r}_1, \mathbf{r}_2) = \frac{1}{N(N-1)} \langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_1) \rangle \quad (4)$$

Here $\langle \dots \rangle = \text{Tr}(\dots \hat{\rho})$ stands for the statistical average over the state $\hat{\rho}$. The density matrix ρ_2 is normalized, namely

$$\text{Tr} \rho_2 = \int_V d^3 r_1 d^3 r_2 \rho_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1, \mathbf{r}_2) = 1,$$

therefore, any matrix element (4) has asymptotic behaviour as $1/V^2$, in the thermodynamic limit $V \rightarrow \infty$, $N/V = n = \text{const}$. Therefore, it is more convenient to work with the pair correlation function

$$F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = \langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_1) \rangle. \quad (5)$$

The boundary conditions for F_2 [22] follow from the principle of the correlation weakening at macroscopical separations [9]:

$$\begin{aligned} \langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_1) \rangle \rightarrow \\ \langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \rangle \langle \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_1) \rangle \end{aligned} \quad (6)$$

when

$$\mathbf{r}_1 - \mathbf{r}_2 = \text{const}, \mathbf{r}'_1 - \mathbf{r}'_2 = \text{const}, |\mathbf{r}'_1 - \mathbf{r}_1| \rightarrow \infty; \quad (7)$$

$$\begin{aligned} \langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_1) \rangle \rightarrow \\ \langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}(\mathbf{r}'_1) \rangle \langle \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}'_2) \rangle \end{aligned} \quad (8)$$

when

$$\mathbf{r}_1 - \mathbf{r}'_1 = \text{const}, \mathbf{r}_2 - \mathbf{r}'_2 = \text{const}, |\mathbf{r}_1 - \mathbf{r}_2| \rightarrow \infty. \quad (9)$$

It should be stressed that limits (6) and (8) are valid either the Bose-Einstein condensation takes place or not. In the first case the anomalous averages in the expression (6) are not zero [23].

As the expression (5) is a Hermitian kernel, we can expand it in the orthonormal set of its eigenprojectors (in the Hilbert space):

$$F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = \sum_{\nu} N_{\nu} \Psi_{\nu}^*(\mathbf{r}_1, \mathbf{r}_2) \Psi_{\nu}(\mathbf{r}'_1, \mathbf{r}'_2) \quad (10)$$

where

$$\int_V d^3 r_1 d^3 r_2 |\Psi_{\nu}(\mathbf{r}_1, \mathbf{r}_2)|^2 = 1. \quad (11)$$

Eigenfunctions $\Psi_{\nu}(\mathbf{r}_1, \mathbf{r}_2)$, which at the same time are eigenfunctions of 2-matrix (4), are called the wave functions of pairs of particles, or PWF. From (5), (10) and (11) we get

$$\begin{aligned} \int_V d^3 r_1 d^3 r_2 F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_1, \mathbf{r}_2) &= \langle \hat{N}^2 - \hat{N} \rangle \\ &= N(N-1) = \sum_{\nu} N_{\nu}, \end{aligned}$$

i.e. the sum of all N_{ν} is the total number of pairs. Therefore, the non-negative quantities N_{ν} can be interpreted as the mean number of the pairs in the state ν , any pair being doubly taken. The ratio $w_{\nu} = N_{\nu}/[N(N-1)]$ is the probability of observing a particle pair in the pure state with the wave function $\Psi_{\nu}(\mathbf{r}_1, \mathbf{r}_2)$. Here, as one might expect, $\sum_{\nu} w_{\nu} = 1$.

From the definition (5) it follows that

$$F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = F_2(\mathbf{r}_2, \mathbf{r}_1; \mathbf{r}'_1, \mathbf{r}'_2) = F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_2, \mathbf{r}'_1)$$

hence, $\Psi_{\nu}(\mathbf{r}_1, \mathbf{r}_2) = \Psi_{\nu}(\mathbf{r}_2, \mathbf{r}_1)$, i.e. the PWF for bosons are symmetric with respect to permutations.

For equilibrium states, the momentum of centre of mass of a pair of particles \mathbf{q} is a quantum number corresponding to PWF, so the index ν can be represented as $\nu = (\omega, \mathbf{q})$, where ω stands for other indices. PWF can be written in the following form

$$\Psi_{\nu}(\mathbf{r}_1, \mathbf{r}_2) = \psi_{\omega, \mathbf{q}}(\mathbf{r}_1 - \mathbf{r}_2) \frac{\exp[i\mathbf{q}(\mathbf{r}_1 + \mathbf{r}_2)/2]}{\sqrt{V}}. \quad (12)$$

Let us demonstrate this. Consider an equilibrium state described by the Gibbs canonical ensemble. As the Hamiltonian is invariant under translations, the total momentum \mathbf{P} is conserved. So, we have

$$\Psi_n(\mathbf{r}_1 + \mathbf{a}, \dots, \mathbf{r}_N + \mathbf{a}) = \Psi_n(\mathbf{r}_1, \dots, \mathbf{r}_N) \exp[i\mathbf{P}\mathbf{a}], \quad (13)$$

Without loss of generality we put $\mathbf{P} = 0$, and introduce new variables

$$\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad (14)$$

and similarly for \mathbf{r}'_1 and \mathbf{r}'_2 . Rewrite (2) with the help of (13) setting $\mathbf{a} = \mathbf{R}$ and $\mathbf{a} = \mathbf{R}'$, respectively. Substituting rewritten Eq. (2) into (3) and performing the Fourier transformations with respect to $\mathbf{r}'_3 - \mathbf{R}', \dots, \mathbf{r}'_N - \mathbf{R}', \mathbf{r}_3 - \mathbf{R}, \dots, \mathbf{r}_N - \mathbf{R}$ we obtain:

$$\rho_2(\mathbf{r}'_1, \mathbf{r}'_2, \mathbf{r}_1, \mathbf{r}_2) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}(\mathbf{R}' - \mathbf{R})} \rho_{\mathbf{q}}(\mathbf{r}', \mathbf{r}), \quad (15)$$

where $\rho_{\mathbf{q}}$ is a non-negative Hermitian kernel. Expanding it in the set of its eigenprojectors $\psi_{\omega, \mathbf{q}}(\mathbf{r}') \psi_{\omega, \mathbf{q}}^*(\mathbf{r})$ we arrive at Eqs. (10) and (12). Analogous proof can be given for the Gibbs grand canonical ensemble.

Then the expression (10) can be written in the form

$$\begin{aligned} F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) &= \sum_{\omega, \mathbf{q}} \frac{N_{\omega, \mathbf{q}}}{V} \psi_{\omega, \mathbf{q}}^*(\mathbf{r}_1 - \mathbf{r}_2) \psi_{\omega, \mathbf{q}}(\mathbf{r}'_1 - \mathbf{r}'_2) \\ &\times \exp\left[i\frac{\mathbf{q}}{2}(\mathbf{r}'_1 + \mathbf{r}'_2 - \mathbf{r}_1 - \mathbf{r}_2)\right]. \end{aligned} \quad (16)$$

For $\psi_{\omega, \mathbf{q}}(\mathbf{r})$, which can be interpreted as the wave function of a pair of particles in the centre-of-mass system, from (11) and (12) we get the following normalization condition:

$$\int_V d^3r |\psi_{\omega,\mathbf{q}}(\mathbf{r})|^2 = 1. \quad (17)$$

As the wave function $\psi_{\omega,\mathbf{q}}(\mathbf{r})$ is an EF of the kernel $\rho_{\mathbf{q}}(\mathbf{r}', \mathbf{r})$ (see Eq. (15)), it can belong either to a discrete or a continuous spectrum, so we have two possible situations [24]:

(1) $\psi_{\omega,\mathbf{q}}(\mathbf{r}) \rightarrow 0$ at $r \rightarrow \infty$ (bound state of a pair of particles).

(2) $\psi_{\omega,\mathbf{q}}(\mathbf{r}) \rightarrow \sqrt{2} \cos(\mathbf{p}\mathbf{r})$ at $r \rightarrow \infty$ (“dissociated” states of a pair of particles corresponding to scattering with relative momentum \mathbf{p} , the factor $\sqrt{2}$ stands for the appropriate normalization when $p \neq 0$).

In the first case, $\omega = i$ is a discrete index numbering bound pair states. We denote $\psi_{\omega,\mathbf{q}}(\mathbf{r}) = \varphi_{\mathbf{q},i}(\mathbf{r})$ and keep the normalization (17):

$$\int_V d^3r |\varphi_{\mathbf{q},i}(\mathbf{r})|^2 = 1. \quad (18)$$

In the second case [25], $\omega = \mathbf{p}$ and

$$\psi_{\omega,\mathbf{q}}(\mathbf{r}) = \frac{\varphi_{\mathbf{p},\mathbf{q}}(\mathbf{r})}{\sqrt{V}}.$$

Due to Eq. (17) we obtain the normalization

$$\frac{1}{V} \int_V d^3r |\varphi_{\mathbf{p},\mathbf{q}}(\mathbf{r})|^2 = 1. \quad (19)$$

With the variables (14) the expression (16) can be rewritten in the following form:

$$\begin{aligned} F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) &= F_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') = \sum_{\mathbf{q}, i} \frac{N_{q,i}}{V} \varphi_{\mathbf{q},i}^*(\mathbf{r}) \varphi_{\mathbf{q},i}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})] \\ &+ \sum_{\mathbf{p}, \mathbf{q}} \frac{N_{\mathbf{p},\mathbf{q}}}{V^2} \varphi_{\mathbf{p},\mathbf{q}}^*(\mathbf{r}) \varphi_{\mathbf{p},\mathbf{q}}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})]. \end{aligned} \quad (20)$$

In the limit $V \rightarrow \infty$ we should replace the quasidiscrete momentum sums by the corresponding integrals:

$$\begin{aligned} F_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') &= \sum_i \int d^3q w_i(q) \varphi_{\mathbf{q},i}^*(\mathbf{r}) \varphi_{\mathbf{q},i}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})] \\ &+ \int d^3p d^3q w(\mathbf{p}, \mathbf{q}) \varphi_{\mathbf{p},\mathbf{q}}^*(\mathbf{r}) \varphi_{\mathbf{p},\mathbf{q}}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})]. \end{aligned} \quad (21)$$

Thus, one can see from Eqs. (20), (21) that $V w_i(q) d^3q$ is the number of bound pairs in state i with momentum \mathbf{q} in an infinitesimally small momentum volume d^3q , and $V^2 w(\mathbf{p}, \mathbf{q}) d^3p d^3q$ is the number of “dissociated”, or scattered, pairs with relative momentum \mathbf{p} and centre-of-mass momentum \mathbf{q} in infinitesimally small momentum volumes d^3p and d^3q .

In the centre-of-mass system the replacement $\mathbf{p} \rightarrow -\mathbf{p}$ corresponds to the permutation of particles. So, the following symmetric relations take place:

$$w(\mathbf{p}, \mathbf{q}) = w(-\mathbf{p}, \mathbf{q}), \quad (22)$$

$$\varphi_{\mathbf{p},\mathbf{q}}(\mathbf{r}) = \varphi_{\mathbf{p},\mathbf{q}}(-\mathbf{r}) = \varphi_{-\mathbf{p},\mathbf{q}}(\mathbf{r}). \quad (23)$$

Let us now prove, with the principle of the correlation weakening, that the distribution of the particle pairs over the “scattering” states $w(\mathbf{p}, \mathbf{q})$ is expressed in terms of the single-particle momentum distribution $w_{sing}(\mathbf{k}) = n_0 \delta(\mathbf{k}) + n(k)/(2\pi)^3$, where $\delta(\mathbf{k})$ stands for the 3-dimensional δ -function, $n(k) = \langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \rangle$ is the single-particle occupation number. Suppose that the temperature is larger than the temperature of the Bose-Einstein condensation, so, $n_0 = 0$ and $w_{sing}(k)$ is a regular function, i.e. it does not contain δ -function after the thermodynamic limit. On the one hand, in the limiting situation of (9) we have the relation (8), which can be written as

$$\begin{aligned} F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) &\rightarrow \int \frac{d^3p_1}{(2\pi)^3} n(p_1) \exp[i\mathbf{p}_1(\mathbf{r}'_1 - \mathbf{r}_1)] \int \frac{d^3p_2}{(2\pi)^3} n(p_2) \exp[i\mathbf{p}_2(\mathbf{r}'_2 - \mathbf{r}_2)] \\ &= \int d^3q d^3p \frac{n(\mathbf{q}/2 + \mathbf{p}) n(\mathbf{q}/2 - \mathbf{p})}{(2\pi)^6} \exp[i\mathbf{p}(\mathbf{r}' - \mathbf{r})] \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})], \end{aligned} \quad (24)$$

where, passing to the last equality, we introduced the new variables $\mathbf{q} = \mathbf{p}_1 + \mathbf{p}_2$ and $\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2$ and used notations (14). On the other hand, when (9) is true, we have

$$r = |\mathbf{r}_2 - \mathbf{r}_1| \rightarrow \infty, \quad r' = |\mathbf{r}'_2 - \mathbf{r}'_1| \rightarrow \infty, \quad |\mathbf{r} + \mathbf{r}'| \rightarrow \infty, \quad \mathbf{R}' - \mathbf{R} = \text{const}, \quad \mathbf{r}' - \mathbf{r} = \text{const}.$$

Hence, in this limit we obtain

$$\varphi_{\mathbf{q},i}(\mathbf{r}) \rightarrow 0, \quad \varphi_{\mathbf{p},\mathbf{q}}(\mathbf{r}) \rightarrow \sqrt{2} \cos(\mathbf{p}\mathbf{r}).$$

Therefore, it follows from (21) that in the limiting case (9) we have

$$F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) \rightarrow \int d^3q d^3p w(\mathbf{p}, \mathbf{q}) 2 \cos(\mathbf{p}\mathbf{r}) \cos(\mathbf{p}\mathbf{r}') \times \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})]. \quad (25)$$

Further, the Riemann's theorem [26] used while integrating over \mathbf{p} and relation (22) allow us to rewrite (25) as

$$F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) \rightarrow \int d^3q d^3p w(\mathbf{p}, \mathbf{q}) \exp[i\mathbf{p}(\mathbf{r}' - \mathbf{r})] \times \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})]. \quad (26)$$

The right-hand side of Eq. (24) is equal to that of (26) at all the values of space variables $\tilde{\mathbf{r}} = \mathbf{r}' - \mathbf{r}$ and $\tilde{\mathbf{R}} = \mathbf{R}' - \mathbf{R}$. Hence, we derive the following equality:

$$w(\mathbf{p}, \mathbf{q}) = \frac{n(\mathbf{q}/2 + \mathbf{p})n(\mathbf{q}/2 - \mathbf{p})}{(2\pi)^6}. \quad (27)$$

Below the temperature of the Bose-Einstein condensation a macroscopic number of particles N_0 occupies the zero-momentum state: $n_0 = \langle \hat{a}_0^\dagger \hat{a}_0 \rangle / V = N_0 / V = \text{const}$, when $V \rightarrow \infty$, and we have in the thermodynamic limit

$$\langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}(\mathbf{r}'_1) \rangle = \int d^3p_1 \left(n_0 \delta(\mathbf{p}_1) + \frac{n(p_1)}{(2\pi)^3} \right) \times \exp[i\mathbf{p}_1(\mathbf{r}'_1 - \mathbf{r}_1)].$$

By analogy with the above proof one can readily be convinced that the distribution $w(\mathbf{p}, \mathbf{q}) = w(\frac{\mathbf{p}_1 - \mathbf{p}_2}{2}, \mathbf{p}_1 + \mathbf{p}_2)$ contains the following parts:

$$1) \quad n_0^2 \delta(\mathbf{p}_1) \delta(\mathbf{p}_2), \quad (28)$$

$$2) \quad n_0 \delta(\mathbf{p}_1) \frac{n(p_2)}{(2\pi)^3} + n_0 \delta(\mathbf{p}_2) \frac{n(p_1)}{(2\pi)^3}, \quad (29)$$

$$3) \quad \frac{n(p_1)}{(2\pi)^3} \frac{n(p_2)}{(2\pi)^3}. \quad (30)$$

The expression (28) corresponds to condensate pair states, or condensate-condensate pairs (both particle of a couple are in the condensate); the terms (29), to condensate-supracondensate pairs; and the last term (30), to supracondensate-supracondensate ones. Thus, owing to the expressions (28)-(30) we obtain the natural classification of the “dissociated” pair states.

We note that the total number of bound pairs $N_b \simeq V \sum_i \int d^3q w_i(q)$ is asymptotically proportional to V^1 , while the total number of “dissociated” pairs $N_d \simeq V^2 \int d^3p d^3q w(\mathbf{p}, \mathbf{q}) = N^2$ is asymptotically proportional to V^2 . From an intuitive point of view it is obvious, as a given particle in a liquid can form bound states with

M particles ($M = \text{const}$ as $V \rightarrow \infty$), while it forms “dissociated” states with the other $N - 1 - M$ particles. So, we arrive at the following asymptotic equation:

$$N_b + N_d = N(N - 1) \simeq N_d \simeq N^2.$$

Diagonal elements of $F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2)$ depend on squared absolute values of the PWF and determine the behaviour of the static pair distribution function $g(r)$, which can be directly observed in scattering experiments:

$$g(r) = \frac{V^2}{N(N - 1)} F_2(\mathbf{r}, \mathbf{R}; \mathbf{r}, \mathbf{R}) = \frac{V^2}{N(N - 1)} \sum_{\omega, \mathbf{q}} \frac{N_{\omega, \mathbf{q}}}{V} |\psi_{\omega, \mathbf{q}}(\mathbf{r})|^2.$$

After the thermodynamic limit this expression takes a form

$$g(r) = \frac{1}{n^2} \left(\sum_i \int d^3q w_i(q) |\varphi_{\mathbf{q},i}(\mathbf{r})|^2 + \int d^3p d^3q w(\mathbf{p}, \mathbf{q}) |\varphi_{\mathbf{p},\mathbf{q}}(\mathbf{r})|^2 \right). \quad (31)$$

One can easily be convinced that $g(r) \rightarrow 1$ as $r \rightarrow \infty$. The behaviour of $g(r)$ for $r \rightarrow 0$ is determined by the PWF at small distances. Because of repulsion, the probability of finding three particles in a very small volume is much lower than that of finding two particles in the same volume. Therefore, the short-range behaviour of two particles is determined by the ordinary two-body Schrödinger equation with the pairwise interaction $\Phi(r)$. Thus, the PWF for short distances between two particles is proportional to the usual wave function $\varphi_{\mathbf{p}}^{(0)}(\mathbf{r})$ of the two-body problem [27]:

$$\varphi_{\mathbf{p},\mathbf{q}}(\mathbf{r}) \rightarrow C \varphi_{\mathbf{p}}^{(0)}(\mathbf{r}), \quad (32)$$

when $r \rightarrow 0$. This implies that for a singular potential the PWF goes to zero for $r \rightarrow 0$, and it follows that $g(r) \rightarrow 0$ as $r \rightarrow 0$.

III. STRUCTURE OF PAIR CORRELATION FUNCTION AND PAIR WAVE FUNCTIONS FOR BOSE LIQUID WITH CONDENSATE

In order to examine the behaviour of the pair correlation function (5) with a condensate we will employ the procedure proposed first by Bogoliubov [1] and lately justified with the help of the principle of correlation weakening [9]: in the calculation of averages [28] of any number of the field operators we can substitute the C -number $\sqrt{N_0}$ for the operators \hat{a}_0 and \hat{a}_0^\dagger involved in $\hat{\psi}(\mathbf{r})$ and $\hat{\psi}^\dagger(\mathbf{r})$. Here N_0 is the number of particles in the condensate. It should be stressed that, after Bogoliubov,

this substitution gives *asymptotically exact values* of the averages in the limit $V \rightarrow \infty$ and *does not imply any approximations*. Indeed, we have for any average that involves the operator \hat{a}_0/\sqrt{V} :

$$\lim_{V \rightarrow \infty} \langle \frac{\hat{a}_0}{\sqrt{V}} \cdots \hat{\psi}(\mathbf{r}') \cdots \rangle$$

$$= \lim_{V \rightarrow \infty} \frac{1}{V} \int_V d^3r \langle \hat{\psi}(\mathbf{r}) \cdots \hat{\psi}(\mathbf{r}') \cdots \rangle$$

$$= \lim_{V \rightarrow \infty} \frac{1}{V} \int_V d^3r \langle \hat{\psi}(\mathbf{r}) \rangle \langle \cdots \hat{\psi}(\mathbf{r}') \cdots \rangle = \sqrt{n_0} \langle \cdots \hat{\psi}(\mathbf{r}') \cdots \rangle.$$

Here we use the definition $\langle \hat{\psi}(\mathbf{r}) \rangle = \langle \hat{\psi}^\dagger(\mathbf{r}) \rangle = \sqrt{n_0}$ ($n_0 = N_0/V$ is the density of the condensate) and the

fact that the main contribution to the value of the integral comes from infinitely large r . Thus, we can put

$$\begin{aligned} \hat{\psi}(\mathbf{r}) &= \sqrt{n_0} + \hat{\vartheta}(\mathbf{r}), \\ \hat{\psi}^\dagger(\mathbf{r}) &= \sqrt{n_0} + \hat{\vartheta}^\dagger(\mathbf{r}), \end{aligned} \quad (33)$$

where

$$\begin{aligned} \hat{\vartheta}(\mathbf{r}) &= \frac{1}{\sqrt{V}} \sum_{\mathbf{p} \neq 0} \hat{a}_{\mathbf{p}} e^{i\mathbf{p}\mathbf{r}}, \\ \hat{\vartheta}^\dagger(\mathbf{r}) &= \frac{1}{\sqrt{V}} \sum_{\mathbf{p} \neq 0} \hat{a}_{\mathbf{p}}^\dagger e^{-i\mathbf{p}\mathbf{r}} \end{aligned} \quad (34)$$

are supracondensate field operators. Substituting the expression (33) into (5) and using the relation $\langle \hat{\vartheta}(\mathbf{r}) \rangle = \langle \hat{\vartheta}^\dagger(\mathbf{r}) \rangle = 0$ we obtain

$$F_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = F_2^{(1)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) + F_2^{(2)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) + F_2^{(3)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) + F_2^{(4)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2), \quad (35)$$

where we introduce the notations

$$F_2^{(1)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = n_0^2 + n_0 \langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}^\dagger(\mathbf{r}_2) \rangle + n_0 \langle \hat{\vartheta}(\mathbf{r}_2) \hat{\vartheta}(\mathbf{r}'_1) \rangle, \quad (36)$$

$$F_2^{(2)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = n_0 \left(\langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}(\mathbf{r}'_1) \rangle + \langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}(\mathbf{r}'_2) \rangle + \langle \hat{\vartheta}^\dagger(\mathbf{r}_2) \hat{\vartheta}(\mathbf{r}'_2) \rangle + \langle \hat{\vartheta}^\dagger(\mathbf{r}_2) \hat{\vartheta}(\mathbf{r}'_1) \rangle \right), \quad (37)$$

$$\begin{aligned} F_2^{(3)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) &= \sqrt{n_0} \left(\langle \hat{\vartheta}^\dagger(\mathbf{r}_2) \hat{\vartheta}(\mathbf{r}'_2) \hat{\vartheta}(\mathbf{r}'_1) \rangle + \langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}(\mathbf{r}'_2) \hat{\vartheta}(\mathbf{r}'_1) \rangle \right. \\ &\quad \left. + \langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}^\dagger(\mathbf{r}_2) \hat{\vartheta}(\mathbf{r}'_2) \rangle + \langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}^\dagger(\mathbf{r}_2) \hat{\vartheta}(\mathbf{r}'_1) \rangle \right), \end{aligned} \quad (38)$$

$$F_2^{(4)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = \langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}^\dagger(\mathbf{r}_2) \hat{\vartheta}(\mathbf{r}'_2) \hat{\vartheta}(\mathbf{r}'_1) \rangle. \quad (39)$$

The expressions (36)-(39) can be expanded in systems of projectors (in the Hilbert space). For (36)-(38) the corresponding projectors can be expressed in an explicit form in terms of averages of the creation and destruction Bose operators $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$. For (36) we have

$$F_2^{(1)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = n_0^2 \varphi^*(\mathbf{r}_1 - \mathbf{r}_2) \varphi(\mathbf{r}'_1 - \mathbf{r}'_2) - \langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}^\dagger(\mathbf{r}_2) \rangle \langle \hat{\vartheta}(\mathbf{r}'_2) \hat{\vartheta}(\mathbf{r}'_1) \rangle,$$

where

$$\varphi(r) = 1 + \psi(r), \quad (40)$$

$$\psi(r) = \psi(\mathbf{r}_1 - \mathbf{r}_2) = \psi^*(\mathbf{r}_1 - \mathbf{r}_2) = \langle \hat{\vartheta}(\mathbf{r}_1) \hat{\vartheta}(\mathbf{r}_2) \rangle / n_0 = \frac{1}{(2\pi)^3} \int d^3k \psi(k) e^{i\mathbf{k}\mathbf{r}}, \quad (41)$$

$$\psi(k) = \langle \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} \rangle / n_0. \quad (42)$$

In a similar manner we get

$$F_2^{(2)}(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') = \int d^3p d^3q w^{(1)}(\mathbf{p}, \mathbf{q}) \sqrt{2} \cos(\mathbf{p}\mathbf{r}) \sqrt{2} \cos(\mathbf{p}\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})]. \quad (43)$$

Here

$$w^{(1)}(\mathbf{p}, \mathbf{q}) = 2n_0 \delta(\mathbf{q}/2 - \mathbf{p}) \frac{n(\mathbf{q}/2 + \mathbf{p})}{(2\pi)^3} = 2n_0 \delta(\mathbf{q}/2 - \mathbf{p}) \frac{n(\mathbf{q})}{(2\pi)^3} \quad (44)$$

is the momentum distribution for condensate-supracondensate pairs corresponding to the expression (29).

Performing the Fourier transformations, we reduce $F_2^{(3)}$ to the following form

$$F_2^{(3)}(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') = \int d^3p d^3q w^{(1)}(\mathbf{p}, \mathbf{q}) \left(\psi_{\mathbf{p}}(\mathbf{r}') \sqrt{2} \cos(\mathbf{p}\mathbf{r}) + \psi_{\mathbf{p}}^*(\mathbf{r}) \sqrt{2} \cos(\mathbf{p}\mathbf{r}') \right) \times \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})]. \quad (45)$$

where

$$\psi_{\mathbf{p}}(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d^3k \psi_{\mathbf{p}}(\mathbf{k}) e^{i\mathbf{k}\mathbf{r}}, \quad (46)$$

$$\psi_{\mathbf{p}}(\mathbf{k}) = \psi_{\mathbf{p}}(-\mathbf{k}) = \psi_{-\mathbf{p}}(\mathbf{k}) = \sqrt{N_0} \frac{1}{\sqrt{2n_0}} \frac{\langle \hat{a}_{2\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}+\mathbf{k}} \hat{a}_{\mathbf{p}-\mathbf{k}} \rangle}{n(2p)}. \quad (47)$$

The second equation in (47) is a consequence of the invariance of averages with respect to the transformation $\hat{a}_{\mathbf{k}} \rightarrow \hat{a}_{-\mathbf{k}}$, $\hat{a}_{\mathbf{k}}^\dagger \rightarrow \hat{a}_{-\mathbf{k}}^\dagger$, as the Hamiltonian does not change when the transformation is performed. The factor $\sqrt{N_0}$ compensates the decrease of the average value $\langle \hat{a}_{2\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}+\mathbf{k}} \hat{a}_{\mathbf{p}-\mathbf{k}} \rangle \sim V^{-1/2}$, so, the quantity $\psi_{\mathbf{p}}(\mathbf{k})$ is of order 1 in the limit $V \rightarrow \infty$.

From (46) and (47) we obtain the symmetry properties

$$\psi_{\mathbf{p}}(\mathbf{r}) = \psi_{\mathbf{p}}(-\mathbf{r}) = \psi_{-\mathbf{p}}(\mathbf{r}).$$

Summing the expressions (43) and (45) we get

$$\begin{aligned} F_2^{(2)}(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') + F_2^{(3)}(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') &= \int d^3p d^3q w^{(1)}(\mathbf{p}, \mathbf{q}) \varphi_{\mathbf{p}}^*(\mathbf{r}) \varphi_{\mathbf{p}}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})] \\ &\quad - \int d^3q 2n_0 \frac{n(q)}{(2\pi)^3} \psi_{\mathbf{q}/2}^*(\mathbf{r}) \psi_{\mathbf{q}/2}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})], \end{aligned}$$

where

$$\varphi_{\mathbf{p}}(\mathbf{r}) = \varphi_{-\mathbf{p}}(\mathbf{r}) = \varphi_{\mathbf{p}}(-\mathbf{r}) = \sqrt{2} \cos(\mathbf{p}\mathbf{r}) + \psi_{\mathbf{p}}(\mathbf{r}), \quad (48)$$

in accordance with (23).

Now it is not difficult to express (35) in a form similar to (21)

$$F_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') = n_0^2 \varphi^*(r) \varphi(r') + \int d^3p d^3q 2n_0 \delta(\mathbf{q}/2 - \mathbf{p}) \frac{n(q)}{(2\pi)^3} \varphi_{\mathbf{p}}^*(\mathbf{r}) \varphi_{\mathbf{p}}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})] + \tilde{F}_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}'), \quad (49)$$

where

$$\begin{aligned} \tilde{F}_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') &= \tilde{F}_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = F_2^{(4)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) - \langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \rangle \langle \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_1) \rangle \\ &\quad - \int d^3q 2n_0 \frac{n(q)}{(2\pi)^3} \psi_{\mathbf{q}/2}^*(\mathbf{r}) \psi_{\mathbf{q}/2}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})]. \end{aligned} \quad (50)$$

As it is proved in Sec. II, the eigenvalues of $F_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}')$ are given by Eqs. (28)-(30). So, one can conclude that the projectors $\varphi^*(r) \varphi(r')$ and $\varphi_{\mathbf{q}/2}^*(\mathbf{r}) \exp[-i\mathbf{q}\mathbf{R}] \varphi_{\mathbf{q}/2}(\mathbf{r}') \exp[i\mathbf{q}\mathbf{R}']$ are nothing else but the eigenprojectors for the pair correlation function, and, hence, $\varphi(r)$ and $\varphi_{\mathbf{q}/2}(\mathbf{r}) \exp[i\mathbf{q}\mathbf{R}]$ are the PWF for the Bose system below T_c . The first term in (49) corresponds to pairs in the condensate; the second, to condensate-supracondensate pairs; the last one, \tilde{F}_2 , to pairs in the supracondensate, and, maybe, to bound pairs. The PWF $\varphi(r)$ and $\varphi_{\mathbf{p}}(\mathbf{r})$ given by expressions (40)-(42) and (46)-(48) respectively are normalized in accordance with (19). The condensate PWF differs essentially from 1 at short distances and goes to 1 when distances between particles in a pair increase. The situation is similar to the scattering of two bare particles with zero momenta at infinity. The anomalous averages

$\langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \rangle$ in PWF (40) have essentially different physical interpretation in comparison with the fermion systems: they determine the “scattering” part of the condensate PWF, while for fermion systems anomalous averages $\langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \rangle$ themselves are PWF for the bound state of pairs of particles with zero momentum [9,31].

In the condensate-supracondensate PWF (48) we drop the index corresponding to the centre-of-mass momentum as $\mathbf{q} = \pm 2\mathbf{p}$. This is a consequence of the δ -function being present in the pair momentum distribution (44). For the same reason in the condensate-condensate PWF (40) the indices are omitted at all.

The functions $\psi(r)$ and $\psi_{\mathbf{p}}(\mathbf{r})$ defined by Eqs. (41) and (46) are responsible for particle short-distance correlations, therefore, owing to (32) for strongly singular potentials we have

$$\psi(r=0) = -1, \quad \psi_{\mathbf{p}}(\mathbf{r}=0) = -\sqrt{2}, \quad (51)$$

(see the discussion at the end of Sec. II).

It should be emphasized that the pair correlation function for supracondensate particles is \tilde{F}_2 rather than $F_2^{(4)}$ defined by Eq. (39). Since the kernel (49) is non-negative, the kernel (50) is also non-negative. Consequently, the last two terms in the expression for \tilde{F}_2 are reduced to zero by the terms in $F_2^{(4)}$. These terms look like those corresponding to bound states of pairs. If the kernel $F_2^{(4)}$ written in form (21) contains other terms associated with bound states, then the latter are also contained in \tilde{F}_2 and, consequently, in the final expression (49). The distribution over supracondensate-supracondensate pair states is given by the expression (30), and thus, we arrive at the final formula for \tilde{F}_2 :

$$\begin{aligned} \tilde{F}_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') &= \sum_i \int d^3q w_i(q) \varphi_{\mathbf{q},i}^*(\mathbf{r}) \varphi_{\mathbf{q},i}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})] \\ &+ \int d^3p d^3q \frac{n(\mathbf{q}/2 + \mathbf{p})}{(2\pi)^3} \frac{n(\mathbf{q}/2 - \mathbf{p})}{(2\pi)^3} \\ &\times \varphi_{\mathbf{p},\mathbf{q}}^*(\mathbf{r}) \varphi_{\mathbf{p},\mathbf{q}}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})], \end{aligned} \quad (52)$$

where the symmetry properties (23) are fulfilled. Thus, in order to answer the question about real bound states of pairs of particles, one must carry out a detailed analysis taking into account all groups of the terms (36)-(39). We emphasize that we do not specify the size of the bound pairs [the characteristic range of the PWF $\varphi_{\mathbf{q},i}(\mathbf{r})$]. If it is much more than the mean distance between particles, then, following Bogoliubov [9], one may call these pairs “quasi-molecules” [29]. If the radius of the bound particle couples is of the order of the mean distance between particles or, even, less then one may speak about ordinary molecules. Note that “quasi-molecules” are not stable for a Bose system within the mean-field variational treatment [30] which is equivalent to the HFB approach. It is a difficult question whether it is the case beyond the mean-field approximation, so, *a priori* we cannot ignore existence of “quasi-molecules”. The bound pair states

can totally be a result of the collective effects, as in the case of Fermi systems [31]. We note that such situation can even be realized in the case of three particles [32].

It is not difficult to see with the help of the Riemann theorem [26] that the boundary condition (6) is satisfied for (49), (52) in the limit (7).

The expressions (36)-(39) can be interpreted in the conventional way, in terms of scattering processes for pairs of particles $(\mathbf{p}_1, \mathbf{p}_2) \rightarrow (\mathbf{p}'_1, \mathbf{p}'_2)$, where $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}'_1$ and \mathbf{p}'_2 are the particle momenta. For this purpose one should calculate the averages in the momentum representation, i.e. make Fourier transformation. This procedure corresponds to expansion of the PWF in plane waves. Thus, the first term in (36) is related to $\mathbf{p}_1 = \mathbf{p}_2 = \mathbf{p}'_1 = \mathbf{p}'_2 = 0$; the second one, to $\mathbf{p}_1, \mathbf{p}_2 \neq 0$ and $\mathbf{p}'_1 = \mathbf{p}'_2 = 0$; and so on. The terms in (38) correspond to processes when one of the four momenta is zero. These processes become dominant in the vicinity of T_c [33], when $N_0/N \ll 1$. In this case $(\frac{N_0}{N})^2 \ll \frac{N_0}{N} \ll \sqrt{\frac{N_0}{N}}$, so one can expect that $F_2^{(3)}$ is important in the expression (35). Taking into account that the thermodynamic potential is tightly connected with the correlation function, one can assume that the terms in (38) are important to obtain correct thermodynamics at those temperatures. Recall that these are precisely the terms being responsible for the short-range correlations for the condensate-supracondensate pairs.

IV. PAIR WAVE FUNCTIONS IN HARTREE-FOCK-BOGOLIUBOV AND BOGOLIUBOV MODELS

Let us consider the HFB approach from the point of view of PWF. In the HFB method (see the detailed discussion in Ref. [4]), a Hamiltonian is approximated by a quadratic form of the Bose operators $\hat{a}_{\mathbf{p}}^\dagger$ and $\hat{a}_{\mathbf{p}}$ connected with initial operators $\hat{a}_{\mathbf{p}}^\dagger$ and $\hat{a}_{\mathbf{p}}$ by the canonical Bogoliubov transformations. Consequently, all averages can be calculated with the Wick-Bloch-De Dominicis theorem [34]. Thus, we have

$$F_2^{(3)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = 0, \quad (53)$$

$$F_2^{(4)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2) = \langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}(\mathbf{r}'_1) \rangle \langle \hat{\vartheta}^\dagger(\mathbf{r}_2) \hat{\vartheta}(\mathbf{r}'_2) \rangle + \langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}(\mathbf{r}'_2) \rangle \langle \hat{\vartheta}^\dagger(\mathbf{r}_2) \hat{\vartheta}(\mathbf{r}'_1) \rangle + \langle \hat{\vartheta}^\dagger(\mathbf{r}_1) \hat{\vartheta}(\mathbf{r}_2) \rangle \langle \hat{\vartheta}(\mathbf{r}'_2) \hat{\vartheta}^\dagger(\mathbf{r}'_1) \rangle. \quad (54)$$

The correlation function (35) can easily be rewritten in the following form

$$\begin{aligned} F_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') &= n_0^2 \varphi^*(r) \varphi(r') + \int d^3p d^3q \left[2n_0 \delta(\mathbf{q}/2 - \mathbf{p}) \frac{n(q)}{(2\pi)^3} + \frac{n(\mathbf{q}/2 + \mathbf{p})}{(2\pi)^3} \frac{n(\mathbf{q}/2 - \mathbf{p})}{(2\pi)^3} \right] \\ &\times \sqrt{2} \cos(\mathbf{p}\mathbf{r}) \sqrt{2} \cos(\mathbf{p}\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})], \end{aligned} \quad (55)$$

where $\varphi(r)$ is related to the averages via (40). In so doing, $n(p)$ and $\psi(k)$ are expressed in terms of Hamiltonian parameters in a self-consistent manner. From (55) one can see that there are no bound states of particles in the framework of the HFB approach. We note that the expression (55) corresponds to the ideal Bose gas when $\varphi(r) = 1$ and $n(p)$ is the Bose-Einstein distribution with a zero chemical potential. One can see that in this case all PWF are symmetrized plane waves, as it is to be expected.

In the HFB method, only the condensate PWF differs from the plane wave. Since PWF are intimately related to the excitation spectrum, one can assume that it is a rough approximation, which has led to the unphysical gap in the single-particle excitation energy. As Eq. (53) is fulfilled for all temperatures, then the HFB model cannot correctly describe the thermodynamic behaviour of the system in the vicinity of T_c ($T < T_c$). It should be pointed out that the expression (55) is valid provided $n_0 \neq 0$. If $n_0 = 0$, but $\langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \rangle \neq 0$, as in the theory of Valatin and Butler [35] (see the careful analysis by Nozières and Saint James [30]), then $F_2^{(1)} = F_2^{(2)} = F_2^{(3)} = 0$ and $F_2^{(4)}$ is determined by (54). In this case the anomalous averages really correspond to the bound pairs of particles with $q = 0$:

$$F_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') = \rho_0 \varphi^*(r) \varphi(r') + \int d^3p d^3q \frac{n(\mathbf{q}/2 + \mathbf{p})}{(2\pi)^3} \frac{n(\mathbf{q}/2 - \mathbf{p})}{(2\pi)^3} \sqrt{2} \cos(\mathbf{p}\mathbf{r}) \sqrt{2} \cos(\mathbf{p}\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})],$$

where ρ_0 is the density of the bound pairs

$$\rho_0 = \int d^3r_1 |\langle \hat{\psi}(\mathbf{r}_1) \hat{\psi}(\mathbf{r}_2) \rangle|^2,$$

and $\varphi(\mathbf{r}_1 - \mathbf{r}_2) = \langle \hat{\psi}(\mathbf{r}_1) \hat{\psi}(\mathbf{r}_2) \rangle / \sqrt{\rho_0}$ is PWF normalized in accordance with (18) [36].

The Bogoliubov theory of weakly imperfect Bose gas is a particular case of the HFB theory when the condensate depletion is small: $(n - n_0)/n \ll 1$. It can be obtained directly from (35) if we neglect terms of the third and forth orders in $\hat{\psi}$ and $\hat{\psi}^\dagger$ [37]

$$\begin{aligned} F_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') &= n_0^2 \varphi^*(r) \varphi(r') + \int d^3p d^3q 2n_0 \delta(\mathbf{q}/2 - \mathbf{p}) \frac{n(\mathbf{q})}{(2\pi)^3} \\ &\times \sqrt{2} \cos(\mathbf{p}\mathbf{r}) \sqrt{2} \cos(\mathbf{p}\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})]. \end{aligned} \quad (56)$$

Comparing the exact expressions (49) and (52) with Eq. (56) one can reveal that the Bogoliubov model involves the following approximations. First, the supracondensate-supracondensate part is omitted, which is completely justified as the condensate depletion is small. Second, the condensate-supracondensate PWF are symmetrized plane waves [$\psi_{\mathbf{p}}(\mathbf{r}) = 0$ in Eq. (48)], hence, the boundary conditions (51) for a hard-core potential cannot be satisfied by any choice of possible parameters. In particular, the change of the “bare” potential by the effective one leaves this property of the model unaltered. The approximation $\varphi_{\mathbf{p}}(\mathbf{r}) = \sqrt{2} \cos(\mathbf{p}\mathbf{r})$ implies that the Bogoliubov model is nothing else but the ideal gas approximation for the condensate-supracondensate PWF, while the scattering part of the condensate-condensate PWF (41) is not zero but small and can be evaluated within the Born approximation for the in-medium PWF [15,18,38]. Therefore, the Bogoliubov model does not properly take into account the short-range correlations of bosons. So, in the framework of this model we obviously obtain the divergency when evaluating the mean energy for the “bare” hard-core potential due to the infinite contribution of the condensate-supracondensate “channel” involved in the representation (31) to the mean interaction energy per particle (1). The hard-sphere model can be treated as the Bogoliubov model with the replacement $\Phi(r) \rightarrow \delta(\mathbf{r})4\pi a/m$. Even after this substitution we face another divergency. The

point is that the Bogoliubov model involves, in the implicit form, the next-to-Born term for the scattering amplitude: $a_1 = -b$, $b = m/[4\pi(2\pi)^3] \int d^3k \Phi^2(k)/(2T_k)$, where $T_k = k^2/(2m)$. The hard-sphere replacement implies that $\Phi(k) = 4\pi a/m = \text{const}$, which leads to the divergency associated with the parameter b , and, hence, to divergent the mean energy. A cure for this difficulty is to replace the Bogoliubov expression (56) by the exact formula (49) in which the term \tilde{F}_2 can be neglected due to a small condensate depletion:

$$\begin{aligned} F_2(\mathbf{r}, \mathbf{R}; \mathbf{r}', \mathbf{R}') &= n_0^2 \varphi^*(r) \varphi(r') \\ &+ 2n_0 \int \frac{d^3q}{(2\pi)^3} n(q) \varphi_{\mathbf{q}/2}^*(\mathbf{r}) \varphi_{\mathbf{q}/2}(\mathbf{r}') \exp[i\mathbf{q}(\mathbf{R}' - \mathbf{R})]. \end{aligned} \quad (57)$$

In so doing the PWF $\varphi(r)$ and $\varphi_{\mathbf{p}}(\mathbf{r})$ should be determined in a self-consistent manner which provides the boundary conditions (32) [and, hence, (51)]. Along this line with the help of the variational procedure we can derive the following non-linear equation:

$$U(k) = \Phi(k) - \frac{1}{2} \int \frac{d^3q}{(2\pi)^3} \frac{\Phi(|\mathbf{k} - \mathbf{q}|) U(q)}{\sqrt{\tilde{T}_q^2 + 2n\tilde{T}_q} U(q)} \quad (58)$$

valid at zero temperature and small densities [15,18]. Here for the function \tilde{T}_q we can put, within a good accuracy, $\tilde{T}_q \simeq T_q = q^2/(2m)$, $\Phi(k)$ is the Fourier transform of the potential $\Phi(r)$, and $U(k) = \int d^3r \varphi(r) \Phi(r) \exp(-i\mathbf{k}\mathbf{r})$ can be treated as a scattering amplitude in a medium. In the limit $n \rightarrow 0$ Eq. (58) is reduced to the ordinary Lippmann-Schwinger equation for the scattering amplitude which corresponds to the zero scattering momentum. Note that Eq. (58) looks like an equation for the many-body t -matrix $\Gamma(\mathbf{k}, \mathbf{k}', \mathbf{q}; \omega)$ at $\omega = 0$ (see, e.g. the recent review [39], Sec. 4). However, there exist essential differences. First, in general, the equation for the t -matrix is frequency dependent in contrast to Eq. (58). Second, $\Gamma(\mathbf{k}, \mathbf{k}', \mathbf{q}; \omega = 0)$ can not be associated with in-medium scattering amplitude $U_{\mathbf{k}', \mathbf{q}}(\mathbf{k}) = \int d^3r \varphi_{\mathbf{k}', \mathbf{q}}(\mathbf{r}) \Phi(r) \exp(-i\mathbf{k}\mathbf{r})$. In particular, the condensate-supracondensate PWF (46)-(48) is characterized by the index $\mathbf{k}' = \pm \mathbf{q}/2$ and expressed via “triple” averages (47) which are completely neglected in the many-body t -matrix approximation as well as in the Bogoliubov, HFB and Popov ones [39]. Thus, one

cannot associate the PWF $\varphi_{\mathbf{k}',\mathbf{q}}(\mathbf{r})$ with the function $\chi_{\mathbf{k}',\mathbf{q};\omega=0}(\mathbf{r})$ whose Fourier transform is usually defined as $\Gamma(\mathbf{k},\mathbf{k}',\mathbf{q};\omega) = 1/(2\pi)^3 \int d^3p \Phi(p) \chi_{\mathbf{k}',\mathbf{q};\omega}(\mathbf{k}-\mathbf{p})$ [see Ref. [39], Eq. (A.23)]. The latter is often called “effective wave function in a medium”. Third, Eq. (58) is obtained by means of *variational* method *beyond* a mean-field approximation [15,18], while an equation for t -matrix is usually derived by summing a certain set of the diagrams. For this reason the relation $\tilde{T}_q \simeq T_q = q^2/(2m)$ is an approximation for Eq. (58) while the t -matrix formalism deals exactly with T_q . Thus, the relation between the t -matrix and PWF formalism is rather subtle and beyond the scope of this paper. We only note that our definition of the PWF as the eigenfunctions of the 2-matrix is consistent with that of quantum mechanics. Namely, we operate with the functions which determine the average energy of the interaction per particle (1) by means of the representations (31) in accordance with the formalism of quantum statistical mechanics. While the physical sense of the functions $\chi_{\mathbf{k}',\mathbf{q};\omega=0}(\mathbf{r})$ is rather unclear.

At sufficiently large momentum k the main contribu-

tion in the integral in the right-hand side of Eq. (58) comes from the large momenta q . As $\lim_{q \rightarrow \infty} U(q)/\tilde{T}_q = 0$, for $k \rightarrow \infty$ Eq. (58) is also reduced to the two-body Lippmann-Schwinger equation, which leads to the boundary condition (32). However, it follows from Eq. (58) that at finite density n $\psi(k) \propto 1/k$ at small k , and, hence, $\psi(r) \propto 1/r^2$ at $r \rightarrow \infty$, in contrast to the two-body problem which implies $\psi(r) \propto 1/r$. Thus, peculiar overscreening takes place for the condensate-condensate PWF. Details concerning Eq. (58) can be found in Refs. [15,18,19].

With the help of the formalism of the PWF one can obtain the exact relationship between the chemical potential and the PWF (40) and (48) in the presence of the Bose-Einstein condensate. This relationship is of special interest, for it allows us to see in an explicit form how the renormalization of an interatomic interaction takes place as applied to the Gross-Pitaevskii equation, at least in the homogeneous case. Let us consider at first an inhomogeneous Bose system with the Hamiltonian

$$\hat{H} = \int d^3r \hat{\psi}^\dagger(\mathbf{r},t) \left(-\frac{\nabla^2}{2m} + V_{ext}(\mathbf{r}) \right) \hat{\psi}(\mathbf{r},t) + \int d^3r d^3r' \Phi(|\mathbf{r}-\mathbf{r}'|) \hat{\psi}^\dagger(\mathbf{r},t) \hat{\psi}^\dagger(\mathbf{r}',t) \hat{\psi}(\mathbf{r}',t) \hat{\psi}(\mathbf{r},t), \quad (59)$$

where the potential $V_{ext}(\mathbf{r})$ corresponds to the external forces, and $\Phi(r)$ is the “bare” interaction potential. Note that the Bose field operators used in Secs. II and III are related to the zero time: $\psi(\mathbf{r}) = \psi(\mathbf{r},t=0)$, $\psi^\dagger(\mathbf{r}) = \psi^\dagger(\mathbf{r},t=0)$. Using the Heisenberg equation of motion with the Hamiltonian (59) for the Bose field operator $\hat{\psi}(\mathbf{r},t)$ and taking average values we get

$$i \frac{\partial \phi(\mathbf{r},t)}{\partial t} = \left(-\frac{\nabla^2}{2m} + V_{ext}(\mathbf{r}) \right) \phi(\mathbf{r},t) + \int d^3r' \Phi(|\mathbf{r}-\mathbf{r}'|) \langle \hat{\psi}^\dagger(\mathbf{r}',t) \hat{\psi}(\mathbf{r}',t) \hat{\psi}(\mathbf{r},t) \rangle, \quad (60)$$

where $\phi(\mathbf{r},t) = \langle \hat{\psi}(\mathbf{r},t) \rangle$ [and, respectively, $\phi^*(\mathbf{r},t) = \langle \hat{\psi}^\dagger(\mathbf{r},t) \rangle$]. On the other hand, one can make use of the Bogoliubov’s procedure of “extracting” the c -number parts of the Bose field operators in the Hamiltonian (59) (see discussion in Sec. III):

$$\begin{aligned} \hat{\psi}(\mathbf{r},t) &= \phi(\mathbf{r},t) + \hat{\vartheta}(\mathbf{r},t), \\ \hat{\psi}^\dagger(\mathbf{r},t) &= \phi^*(\mathbf{r},t) + \hat{\vartheta}^\dagger(\mathbf{r},t). \end{aligned} \quad (61)$$

Thus, in the stationary equilibrium case the grand canonical potential Ω depends on the c -number complex parameter $\phi(\mathbf{r})$ that can be considered as the order parameter. So, the equilibrium value of the grand canonical potential $\Omega = \Omega(T, V, \mu; \{\phi(\mathbf{r})\}, \{\phi^*(\mathbf{r})\})$ corresponds to a minimum with respect to the order parameter (the parameter μ stands for the chemical potential). Using the well-known expression for an infinitesimal change of the potential $\delta\Omega = \langle \delta(\hat{H} - \mu\hat{N}) \rangle$ one can obtain from the condition $\delta\Omega/\delta\phi(\mathbf{r}) = \delta\Omega/\delta\phi^*(\mathbf{r}) = 0$:

$$\mu\phi(\mathbf{r}) = \left(-\frac{\nabla^2}{2m} + V_{ext}(\mathbf{r}) \right) \phi(\mathbf{r}) + \int d^3r' \Phi(|\mathbf{r}-\mathbf{r}'|) \langle \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \rangle. \quad (62)$$

It is not difficult to see that Eq. (62) is nothing but the stationary form of Eq. (60) corresponding to the solution $\phi(\mathbf{r},t) = \phi(\mathbf{r}) \exp(-i\mu t)$ because in this case we have for the time-dependent “triple” averages

$$\langle \hat{\psi}^\dagger(\mathbf{r}_2,t) \hat{\psi}(\mathbf{r}_2',t) \hat{\psi}(\mathbf{r}_1',t) \rangle = \exp(-i\mu t) \langle \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2') \hat{\psi}(\mathbf{r}_1') \rangle. \quad (63)$$

Indeed, the principle of the correlation weakening requires that at $|\mathbf{r}_1| \rightarrow \infty$

$$\begin{aligned} \langle \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2') \hat{\psi}(\mathbf{r}_1') \rangle &= \langle \hat{\psi}^\dagger(\mathbf{r}_1,t) \hat{\psi}^\dagger(\mathbf{r}_2,t) \hat{\psi}(\mathbf{r}_2',t) \hat{\psi}(\mathbf{r}_1',t) \rangle \rightarrow \\ \langle \hat{\psi}^\dagger(\mathbf{r}_1,t) \rangle \langle \hat{\psi}^\dagger(\mathbf{r}_2,t) \hat{\psi}(\mathbf{r}_2',t) \hat{\psi}(\mathbf{r}_1',t) \rangle &= \langle \hat{\psi}^\dagger(\mathbf{r}_1) \rangle \langle \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2') \hat{\psi}(\mathbf{r}_1') \rangle. \end{aligned}$$

The relation (63) follows from the last equation as $\langle \hat{\psi}^\dagger(\mathbf{r}_1) \rangle = \phi^*(\mathbf{r}_1)$ and $\langle \hat{\psi}^\dagger(\mathbf{r}_1, t) \rangle = \phi^*(\mathbf{r}_1) \exp(i\mu t)$. The stationary Gross-Pitaevskii equation can be obtained from the exact equation (62) with the help of the replacement:

$$\Phi(r) \rightarrow \frac{4\pi a}{m} \delta(\mathbf{r}), \quad (64)$$

$$\langle \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \rangle \rightarrow \phi^*(\mathbf{r}') \phi(\mathbf{r}') \phi(\mathbf{r}), \quad (65)$$

where a is the scattering length which can be defined with the help of the “bare” scattering amplitude: $4\pi a/m = U^{(0)}(0)$ [$U^{(0)}(k)$ is the solution of Eq. (58) at $n = 0$ and $\tilde{T}_q = T_q = q^2/(2m)$]. However, within that approach it is not clear how the renormalization (64) takes place. The most transparent way of understanding this replacement in the homogeneous case is based on the PWF formalism. In this situation $V_{ext}(\mathbf{r}) = 0$, $\phi = \sqrt{n_0} \exp(i\chi)$, and we can put the phase χ equal to zero. So, for the homogeneous system the exact equation (62) reads

$$\mu = \frac{1}{\sqrt{n_0}} \int d^3 r' \Phi(|\mathbf{r} - \mathbf{r}'|) \langle \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \rangle. \quad (66)$$

This equation has been obtained in the momentum representation in the Bogoliubov’s paper [9] (see also Ref. [40]). Using the specific expressions for the scattering parts of the condensate-condensate and supracondensate-condensate PWF given by Eqs. (42) and (47), one can represent Eq. (66) in the following form:

$$\mu = n_0 U(0) + \sqrt{2} \int \frac{d^3 q}{(2\pi)^3} n(q) U_{\mathbf{q}/2}(\mathbf{q}/2), \quad (67)$$

here $U_{\mathbf{p}}(\mathbf{k}) = \int d^3 r \varphi_{\mathbf{p}}(\mathbf{r}) \Phi(r) \exp(-i\mathbf{k}\mathbf{r})$. Equation (67) is the exact representation for the chemical potential via the condensate-condensate and condensate-supracondensate PWF and the occupation numbers $n(k)$. It can be used in order to obtain the density expansion for μ at $n \rightarrow 0$. With the help of the expression for $n(k)$ established within the variational scheme mentioned above [15,18],

$$n(k) = \frac{1}{2} \left(\frac{\tilde{T}_k + nU(k)}{\sqrt{\tilde{T}_k^2 + 2n\tilde{T}_k U(k)}} - 1 \right), \quad (68)$$

one can derive for the condensate density

$$\begin{aligned} n_0 &= n \left(1 - \int \frac{d^3 k}{(2\pi)^3} \frac{n(k)}{n} \right) \\ &= n \left(1 - \frac{8}{3\sqrt{\pi}} \sqrt{na^3} + \dots \right), \end{aligned} \quad (69)$$

where the substitution $\mathbf{k} = \mathbf{k}' \sqrt{2mn}$ in the integral is employed. Besides, at $n \rightarrow 0$ from Eq. (58) one can obtain the density correction for the in-medium scattering amplitude [17–19]

$$U(0) = U^{(0)}(0) \left(1 + \frac{8}{\sqrt{\pi}} \sqrt{na^3} + \dots \right). \quad (70)$$

Using Eqs. (69) and (70) and making the “scaling” substitution $\mathbf{q} = \mathbf{q}' \sqrt{2mn}$ in the integral in Eq. (67), we arrive at the familiar density expansion [10–12]

$$\mu = nU^{(0)}(0) \left(1 + \frac{32}{3\sqrt{\pi}} \sqrt{na^3} + \dots \right). \quad (71)$$

In so doing, the explicit formula for the condensate-supracondensate PWF $\varphi_{\mathbf{p}}(\mathbf{r})$ are needless, but only the relation $\lim_{\mathbf{p} \rightarrow 0} \varphi_{\mathbf{p}}(\mathbf{r}) = \sqrt{2} \varphi(r)$ is of use. The factor $\sqrt{2}$ appears as due to the normalization condition (19).

Now it is not difficult to see that in the homogeneous case the Gross-Pitaevskii equation corresponds to the simplest Hartree approximation with the renormalized potential (64):

$$\mu \simeq n_0 U^{(0)}(0). \quad (72)$$

The range of validity of this approximation is determined by the next-to-leading terms in Eqs. (69)-(71) and readily expressed as $\sqrt{na^3} \ll 1$. In the paper of Prokakis et al. [14] the criterion for validity of the Gross-Pitaevskii equation is formulated as

$$n \frac{4\pi \hbar^2 a}{m} \ll \hbar \omega, \quad (73)$$

where the frequency ω characterizes the harmonic trap potential. In the homogeneous case ($\omega = 0$) it cannot be fulfilled, while the Gross-Pitaevskii approximation (64), (65) is valid, if the condition $\sqrt{na^3} \ll 1$ is realized. Thus, the criterion (73) appears to be refined.

V. SUMMARY

The reduced density matrix of the second order (4) is a fundamental characteristic of a many-particle system, its eigenfunctions, PWF, being the pure states of two particles, selected in an arbitrary way, and its eigenvalues being the probabilities of finding a couple in those states. Thus, the properties of the 2-matrix are of interest in itself and from the point of view of various applications as well.

With the Bogoliubov principle of correlation weakening we express the momentum distribution of “dissociated” pair states in terms of the single-particle occupation numbers [see the expressions (28)-(30)]. This allows us to represent the pair correlation function (5) in the form (49), (52), where the condensate-condensate and condensate-supracondensate PWF are explicitly given by Eqs. (40)-(42) and (46)-(48), respectively. It should be stressed that this representation is exact and do not implies any mean-field approximation as well as various

model assumptions since it is solely based on the Bogoliubov's principle of the correlation weakening. The transparent physical interpretation of the anomalous averages (41) and (46) as the "scattering parts" of the corresponding PWF is proposed. The boundary conditions (51) are obtained in the case of hard-core, or strongly singular, potentials. The condensate-supracondensate PWF is determined by the "triple" average (47). The importance of these averages is emphasized in Ref. [14] for the effects of condensate-excited-state interactions in the evolution of condensate mean field, which are in accordance with our results. In the textbook [41] the crucial role of the contribution of the "triple" averages is discussed in the context of "dielectric formalism" approach. Those averages are not zero in so called Beliaev-Popov approximation discussed recently in [39].

Thus, the anomalous averages $\langle \hat{\vartheta}(\mathbf{r}_1)\hat{\vartheta}(\mathbf{r}_2) \rangle$ are responsible for the spatial correlations of two particles in the condensate, and do not imply that bound states of pairs of particles exist; the terms (38) are found to be responsible for the spatial correlations of condensate-supracondensate pairs of particles and can be expected to be important in thermodynamics near the critical temperature T_c . In the HFB approach, the PWF are symmetrized plane waves except for the condensate pairs provided the condensate density is not equal to zero.

The formalism of PWF is useful to construct various approximations which take into account both short-range and long-range spatial correlations of particles in a self-consistent manner. This is due to the fact that all the pair wave functions in the expansion (49), (52) are "regular channels" from the point of view of its behaviour at small r . Along this line one can obtain the system of non-linear integro-differential equations for PWF, which in the weak-coupling approximation leads to the Bogoliubov model of the weakly interacting Bose gas [38]. For a dilute Bose gas the non-linear integral equation (58) that takes into account both short- and long-range spatial correlations can be obtained with the help of variational method beyond a mean-field approach [17–19]. The exact relationship between PWF and the chemical potential (67) allows us to obtain the density expansion for the chemical potential (71) in the strong-coupling regime (Bose gas is dilute, but the potential is strongly singular as the Lennard-Jones one). In this regime one can derive the expansion for the mean energy per particle in powers of the boson density n , the famous results [11,12] being reproduced without any divergencies which are inherent in the pseudopotential approximation [17–19]. Thus, this expansion can be readily obtained from Eq. (71) with the thermodynamic relation $\mu = \partial(\varepsilon(n))/\partial n$:

$$\varepsilon = \frac{1}{n} \int_0^n dn' \mu(n') = \frac{2\pi\hbar^2 a n}{m} \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{na^3} + \dots \right).$$

Moreover, in the framework of our approach we can obtain by *direct* calculation the interaction energy per par-

ticle (1) (as well as the kinetic one) [17]. However, this is impossible within the effective-potential approach of Refs. [10–12], which obviously indicates the incorrect behaviour of the pair distribution function $g(r)$ (see the detailed discussions in Refs. [17,19]).

It is worth noting that the concept of PWF is helpful not only in the case of the Bose systems but also in the situation of the Fermi ones. Indeed, employing this formalism one can easily prove that below the temperature of the superconducting phase transition there always exist the bound states of fermion pairs beyond the pair condensate [31].

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- $$\begin{aligned} \varphi_{\mathbf{p}, \mathbf{q}, S, m_S}(\mathbf{r}, \sigma_1, \sigma_2) &= \varphi_{\mathbf{p}, \mathbf{q}, S, m_S}(-\mathbf{r}, \sigma_2, \sigma_1) \\ &= \varphi_{-\mathbf{p}, \mathbf{q}, S, m_S}(\mathbf{r}, \sigma_2, \sigma_1), \end{aligned}$$
- where σ_1 and σ_2 are single-particle z -projections of the spin (compare with Eq. (23)). The same is valid for bound states of pairs.
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